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Dispersion of Low-lying Excitations in Half-filled and Doped 1D Hubbard Model

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energy calculated via weak coupling perturbation theory captures reasonably well the binding energy at intermediate coupling. A possible extension of the weak coupling expansion to larger clusters is discussed.

Dispersion of Low-lying Excitations in Half-filled and Doped 1D Hubbard Model

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1. Introduction

Excited states as well as ground state of strongly correlated electron systems have been a subject of intense study in connection with electron mechanisms of the high T_c superconductivity. In one-dimensional(1D) systems one can provide exact results as contrasted with higher dimensional cases in which one has to make such approximations as the strong interaction limit. The exact solution for one class of excitations in 1D was first derived from the Bethe-ansatz solution by des Cloizeaux and Pearson (des Cloizeaux and Pearson 1962, see also Yamada 1969, Faddeev and Takhtajan 1986) for the Heisenberg antiferromagnet. This has been extended to the Hubbard model for the half-filled band (Ovchinnikov 1970, Takahashi 1969, 1970, Woynarovich 1982) and quarter-filled band (Coll 1974). The $U=\infty$ case (Woynarovich 1982, Ogata and Shiba 1990), where U is the Hubbard interaction, and the finite-size effect by conformal field theory (Woynarovich 1989) have also been studied.

In the present study we have numerically obtained the low-lying excitations for single-hole and two-hole states as well as for the half-filled band for various values of U ranging $0 < U < \infty$.

Here the points of interest are the followings:

(i) How does the dispersion of low-lying excitation modes change as one goes from $U=0$ (free electron) to $U=\infty$ (Heisenberg antiferromagnet).

(ii) Although Nagaoka's theorem (Nagaoka 1966, see also Tasaki 1990) does not hold in 1D, can high-spin states emerge, and, if so, what is the dispersion like?

What happens when there are more than one hole?

2. Method

We have obtained the wavefunctions as well as eigenenergies for the ground state and low-lying excited states for finite 1D Hubbard systems by the direct diagonalization

(Lanczos method). The dispersion is obtained by classifying the states by the total spin, S , and the irreducible representation of C_{nv} of the 1D ring. Comparison with the Bethe-ansatz solution is also made.

3. Results

We have first studied the half-filled band (five \uparrow spin and five \downarrow spin electrons on the ten-site chain) for $0.01 < U < 100$. It is shown that des Cloizeaux-Pearson(dCP) mode for $U=\infty$ continuously changes into single-particle excitations across the Fermi level for the $U \rightarrow 0$ fermion system.

If we turn to one-hole system (five \uparrow spin and four \downarrow spin electrons on the ten-site chain), the lowest dispersion comprises the dCP mode and another branch with complex roots in the Bethe-ansatz language. For large U , the dispersion comprises $2t\cos(k/N)$ branch (N : number of electrons), as is pointed out for the $U=\infty$ case (Doucot and Wen 1989).

For two holes (four \uparrow spin and four \downarrow spin electrons for the ten-site chain), the ground state has $S=1$ rather than $S=0$. When the number of sites corresponds to non-closed-shell ($4 \times \text{integer}$), $S=1$ ground state emerges even for the half-filled band (Ogata and Shiba 1990). This can be interpreted as a realization of a generalized Hund's coupling in the k space in finite systems. This k -space Hund's coupling also applies to 2D systems. For large U , the dispersion considerably deviates from the $2t\cos(k/N)$ behaviour when there are more than one hole.

In summary, low-lying excitations in the half-filled and doped 1D Hubbard model exhibit interesting behaviours.

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ハバード $t-J$ 模型におけるホール及びスピンの力学と高温超伝導^(*)

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高温超伝導を記述するミクロスコピックな模型としてハバード $t-J$ 模型を捉え，その物理的性質を理解するために我々が発展させてきた形式化，枠組み，記述法，それらから得られる主な結果について要約した。

我々のアプローチの特徴は，

- ① 電子場をスレーブボソン（スピン）及びフェルミオン（ホール）により表示し，その経路積分により，量子化を行なう。
- ② 近距離ネール秩序を仮定し，奇格子点上のスピン変数について積分する。
- ③ 最近接ホール対を記述する複素リンク変数を超伝導の秩序場として導入する。

主な結果は，

- A 低温における超伝導状態を記述する低エネルギー有効場の理論として，スピン自由度を記述する非線形シグマ模型（複素射影群 CP^1 に植を取る）とホール自由度を記述する相対論的ディラック・フェルミオン模型がゲージ結合した $U(1)$ ゲージ場理論を得る。
- B 超伝導－正常状態間の相転移を記述するギンツブルグーランダウ理論として，上記③のリンク変数をゲージ変数とする $U(1)$ 格子ゲージ・ヒッグス模型を得る。プラケット作用項は J 結合に，ヒッグス作用項は t 結合に起因する。
超伝導はヒッグス相として実現する。
- C 相構造の同定には数値解析が必要だが，一例として，この枠組みによって計算された反強磁性－正常相転移点 (T_N) の結果〔2〕と単純化された可解模型による超伝導－正常相転移点 (T_c) を下図に示す。

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